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INTERNATIONAL PRELIMINARY EXAMINATION REPORT
(PCT Article 36 and Rule 70)

Applicant's or agent's file reference SYN 60002/WO	FOR FURTHER ACTION See Notification of Transmittal of International Preliminary Examination Report (Form PCT/IPEA/416)	
International application No. PCT/GB 03/04921	International filing date *(day/month/year)* 12.11.2003	Priority date *(day/month/year)* 13.11.2002
International Patent Classification (IPC) or both national classification and IPC C08G18/22		
Applicant JOHNSON MATTHEY PLC et al.		

1. This international preliminary examination report has been prepared by this International Preliminary Examining Authority and is transmitted to the applicant according to Article 36.

2. This REPORT consists of a total of 4 sheets, including this cover sheet.

   ☒ This report is also accompanied by ANNEXES, i.e. sheets of the description, claims and/or drawings which have been amended and are the basis for this report and/or sheets containing rectifications made before this Authority (see Rule 70.16 and Section 607 of the Administrative Instructions under the PCT).

   These annexes consist of a total of 4 sheets.

3. This report contains indications relating to the following items:

   - I ☒ Basis of the opinion
   - II ☐ Priority
   - III ☐ Non-establishment of opinion with regard to novelty, inventive step and industrial applicability
   - IV ☐ Lack of unity of invention
   - V ☒ Reasoned statement under Rule 66.2(a)(ii) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement
   - VI ☐ Certain documents cited
   - VII ☐ Certain defects in the international application
   - VIII ☐ Certain observations on the international application

Date of submission of the demand	Date of completion of this report
11.06.2004	25.02.2005
Name and mailing address of the international preliminary examining authority: European Patent Office D-80298 Munich Tel. +49 89 2399 - 0 Tx: 523656 epmu d Fax: +49 89 2399 - 4465	Authorized Officer Krätzschmar, U Telephone No. +49 89 2399-2137

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

International application No. PCT/GB 03/04921

I. Basis of the report

1. With regard to the **elements** of the international application *(Replacement sheets which have been furnished to the receiving Office in response to an invitation under Article 14 are referred to in this report as "originally filed" and are not annexed to this report since they do not contain amendments (Rules 70.16 and 70.17))*:

Description, Pages

1-14 as originally filed

Claims, Numbers

1-18 received on 10.02.2005 with letter of 09.02.2005

2. With regard to the **language**, all the elements marked above were available or furnished to this Authority in the language in which the international application was filed, unless otherwise indicated under this item.

These elements were available or furnished to this Authority in the following language: , which is:

- ☐ the language of a translation furnished for the purposes of the international search (under Rule 23.1(b)).
- ☐ the language of publication of the international application (under Rule 48.3(b)).
- ☐ the language of a translation furnished for the purposes of international preliminary examination (under Rule 55.2 and/or 55.3).

3. With regard to any **nucleotide and/or amino acid sequence** disclosed in the international application, the international preliminary examination was carried out on the basis of the sequence listing:

- ☐ contained in the international application in written form.
- ☐ filed together with the international application in computer readable form.
- ☐ furnished subsequently to this Authority in written form.
- ☐ furnished subsequently to this Authority in computer readable form.
- ☐ The statement that the subsequently furnished written sequence listing does not go beyond the disclosure in the international application as filed has been furnished.
- ☐ The statement that the information recorded in computer readable form is identical to the written sequence listing has been furnished.

4. The amendments have resulted in the cancellation of:

- ☐ the description, pages:
- ☐ the claims, Nos.:
- ☐ the drawings, sheets:

5. ☐ This report has been established as if (some of) the amendments had not been made, since they have been considered to go beyond the disclosure as filed (Rule 70.2(c)).

(Any replacement sheet containing such amendments must be referred to under item 1 and annexed to this report.)

6. Additional observations, if necessary:

V. Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

1. Statement

Novelty (N)	Yes:	Claims	1-18
	No:	Claims	
Inventive step (IS)	Yes:	Claims	1-18
	No:	Claims	
Industrial applicability (IA)	Yes:	Claims	1-18
	No:	Claims	

2. Citations and explanations

see separate sheet

Ad section V.:

1. Novelty (Art. 33(2) PCT):

   The subject-matter of present claims 1 to 18 is considered to be novel over the available prior art.
   None of the documents discloses an organometallic compound having the specific structure according to present claim 1 and its use as a cure catalyst in the preparation of polyurethanes.

2. Inventive step (Art. 33(3) PCT):

   The subject-matter of claims 1-18 is also considered as involving an inventive step. Document US-A-5 902 835 (D2) which is taken as the closest prior art discloses a catalyst system for the preparation of polyurethane foams including a specific Group IVB metal blowing catalyst (see claims 1 and 10). D2 teaches that the catalyst activity and its selectivity to blowing or gelling is very much dependent upon the ligands that are coordinated to the metals (see col.15, l.6 - col.16,l.7 and table 2). D2 does not suggest that the specific structure of the organometallic compound according to present claim 1 gives very effective polyurethane cure catalysts which can be used even in smaller quantities than the commercial mercury-based catalysts (see example 14 and results in table 1).

3. The description has not been adapted to the new set of claims. Examples 1 and 2 not falling under the scope of present claim 1 have to be designated as comparative examples.

Claims

1. An organometallic compound of formula $RO\text{-}M(L^1)_x(L^2)_y(L^3)_z$

wherein M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;

R is alkyl or a hydroxy-alkyl, hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, and

(i) when R is alkyl, L^1 and L^2 are each independently selected from a β-diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof or siloxy,

(ii) when R is a hydroxy-alkyl hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, L^1 and L^2 are each independently selected from a diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R^1COO- where R^1 is substituted or unsubstituted $C_1 - C_{30}$ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonato;

in both case (i) and case(ii), provided that when L^1 is a ligand which forms two covalent bonds with the metal atom, and x = 1 then y = 0;

L^3 is selected from substituted or unsubstituted phenol or naphthol, R^2COO- where R^2 is a linear or branched $C_1 - C_{30}$ alkyl or benzene, a polyoxyalkoxy or hydroxyalkoxyalkoxy group;

x and y are each either 0 or 1,

z=1

$(x+y+z) \leq V-1$, where V= the valency of the metal M.

2. An organometallic compound according to claim 1, wherein R is a $C_1 - C_8$ alkyl group or a hydroxy-alkyl group derived from a diol.

3. An organometallic compound according to claim 2, wherein R is selected from the group consisting of ethyl, n-propyl, isopropyl, n-butyl, t-butyl, pentyl, hexyl, hydroxybutyl, polyoxyethyl and 2-(2-hydroxyethoxy)-ethyl.

4. An organometallic compound according to any one of claims 1 – 3, wherein L^1 and L^2 are selected from acetyl acetone, an alkylacetoacetate, an N-alkylacetoacetamide, salicylic acid or ester thereof, mandelic acid or ester thereof, levulinic acid or ester thereof, or naphthalene dicarboxylic acid or ester thereof.

5. An organometallic compound according to any one of claims 1 – 4, wherein L^3 is selected from the group consisting of substituted or unsubstituted phenol or naphthol, or a $C_2 - C_{30}$ carboxylic acid.

6. A cure catalyst composition, suitable for catalysing the formation of urethane bonds, comprising a mixture of an organometallic compound according to any one of claims 1 – 5 and an acid.

7. A cure catalyst composition according to claim 6, wherein said organometallic compound and said acid are mixed together in a mole ratio of from 0.1 to 10 moles of acid per mole of organometallic compound.

8. A cure catalyst composition according to either claim 6 or claim 7, wherein the acid is a $C_2 - C_{30}$ carboxylic acid.

9. A composition comprising:

a) either

i) a compound having more than one hydroxy group which is capable of reacting with an isocyanate group -containing material to form a polyurethane or

ii) a compound having more than one isocyanate group which is capable of reacting with a hydroxyl group-containing material to form a polyurethane,

b) an organometallic compound of formula $RO\text{-}M(L^1)_x(L^2)_y(L^3)_z$

wherein M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;

R is alkyl or a hydroxy-alkyl, hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, and

(i) when R is alkyl, L^1 and L^2 are each independently selected from a β-diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof or siloxy,

(ii) when R is a hydroxy-alkyl hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, L^1 and L^2 are each independently selected from a diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R^1COO- where R^1 is substituted or unsubstituted $C_1 - C_{30}$ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonato;

in both case (i) and case(ii), provided that when L^1 is a ligand which forms two covalent bonds with the metal atom, and $x = 1$ then $y = 0$;

L^3 is selected from substituted or unsubstituted phenol or naphthol, R^2COO- where R^2 is a linear or branched $C_1 - C_{30}$ alkyl or benzene, a polyoxyalkoxy or hydroxyalkoxyalkoxy group;

x and y are each either 0 or 1,

$z=1$

$(x+y+z) \leq V-1$, where V= the valency of the metal M; and optionally

c) one or more further components selected from chain modifiers, diluents, flame retardants, blowing agents, release agents, water, coupling agents, lignocellulosic preserving agents, fungicides, waxes, sizing agents, fillers, colourants, impact modifiers, surfactants, thixotropic agents, flame retardants, plasticisers, and other binders.

10. A composition according to claim 9, wherein when R is alkyl, L^1 and L^2 are each independently selected from a β-diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, or siloxy.

11. A composition according to claim 10, further comprising an acid.

12. A composition according to claim 11, wherein the acid is intimately mixed with the organometallic compound of component b).

13. A composition according to claim 11, wherein the acid is a $C_2 - C_{30}$ carboxylic acid.

14. A process for manufacturing an organometallic composition, comprising reacting together:-
(a) a metal alkoxide, having a formula $M(OR)_V$, where:
M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;
V= the valency of the metal M, and
R is alkyl, and
(b) a β-diketone, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R^1COO- where R^1 is substituted or unsubstituted $C_1 - C_{30}$ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonato; in an amount to provide about 1 or 2 moles of component (b) per mole of metal M in component (a); and
(c) a substituted or unsubstituted aryloxy, R^2COO- where R^2 is a linear or branched $C_1 - C_{30}$ alkyl or a substituted or unsubstituted aryl, a polyoxyalkylalcohol or hydroxyalkoxyalcohol in an amount to provide about 1 mole of component (c) per mole of metal M in component (a);
(d) optionally removing alcohol ROH formed during the reaction of (a) with (b) and (c).

15. A process as claimed in claim 14 for manufacturing an organometallic compound according to any of claims 1 – 5.

16. A process as claimed in claim 14 or claim 15, wherein the metal alkoxide $M(OR)_V$ is first reacted with one of component (b) or component (c) and then with the other of components (b) or (c) and the alcohol ROH formed during the reaction of the alkoxide with components (b) and (c) is removed after each reaction step.

17 A process as claimed in any of claims 14 to 16, wherein the product is further reacted with a hydroxy-functionalised alcohol which is preferably a hydroxy-alcohol, hydroxyalkoxyalcohol, or (hydroxy)polyoxyalkylalcohol and a further quantity of ROH is removed from the reaction mixture.

18. A process for the manufacture of a polyurethane article, comprising the steps of :

a) forming a mixture by mixing together either

i) a compound having more than one hydroxy group which is capable of reacting with an isocyanate group -containing material to form a polyurethane or

ii) a compound having more than one isocyanate group which is capable of reacting with a hydroxyl group-containing material to form a polyurethane,

with an organometallic compound of formula $RO\text{-}M(L^1)_x(L^2)_y(L^3)_z$

wherein M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;

L^1 and L^2 are each independently selected from a diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R^1COO- where R^1 is substituted or unsubstituted $C_5 - C_{30}$ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonato, provided that when L^1 is a ligand which forms two covalent bonds with the metal atom, and $x = 1$ then $y = 0$;

L^3 is selected from substituted or unsubstituted aryloxy, R^2COO- where R^2 is a linear or branched $C_6 - C_{30}$ alkyl, and a polyoxyalkyl or hydroxyalkoxyalkyl group;

R is alkyl or hydroxy-alkyl hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group,

x, y and z are each either 0 or 1

$(x+y+z) \leq V-1$, where V= the valency of the metal M;

b) adding to said mixture the other of the compound having more than one hydroxy group which is capable of reacting with an isocyanate group -containing material to form a polyurethane or the a compound having more than one isocyanate group which is capable of reacting with a hydroxyl group-containing material to form a polyurethane,

c) forming said mixture into the required shape for the polyurethane article,

d) allowing said mixture to cure

e) optionally subjecting the mixture to specified conditions for post-cure conditioning.